

Journal of

Computational Physics

VOLUME 47, 1982



ACADEMIC PRESS

Subsidiary of Harcourt Brace Jovanovich, Publishers

**New York London
Paris San Diego San Francisco São Paulo Sydney Tokyo Toronto**

Copyright © 1982 by Academic Press, Inc.

All Rights Reserved

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

The appearance of the code at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (21 Congress Street, Salem, Massachusetts 01970), for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-1982 articles are the same as those shown for current articles.

CONTENTS OF VOLUME 47

NUMBER 1, JULY 1982

REVIEW ARTICLE

JOE F. THOMPSON, ZAHIR U. A. WARSI, AND C. WAYNE MASTIN. Boundary-Fitted Coordinate Systems for Numerical Solution of Partial Differential Equations—A Review	1
WING L. CHAN AND CHARLES L. WOLF. ADI on Staggered Mesh—a Method for the Calculation of Compressible Convection	109
ICHIO KUMAGAI. A Numerical Study of Wind-Driven Circulation in Rectangular Cavities	130
CORNILLE. A Pseudospectral Scheme for the Numerical Calculation of Shocks	146

LETTER

ANDERS SKÖLLERMO. A Better Difference Scheme for the Laplace Equation in Cylindrical Coordinates	160
ST OF FORTHCOMING ARTICLES	164

NUMBER 2, AUGUST 1982

S. PAWLEY AND G. W. THOMAS. The Implementation of Lattice Calculations on the DAP	165
S. BRAMLEY AND S. C. R. DENNIS. The Calculation of Eigenvalues for the Stationary Perturbation of Poiseuille Flow	179
M. SANZ-SERNA. An Explicit Finite-Difference Scheme with Exact Conservation Properties	199
ER LÖTSTEDT. A Front Tracking Method Applied to Burgers' Equation and Two-Phase Porous Flow	211
C. ADAM, A. GOURDIN SERVENIERE, AND A. B. LANGDON. Electron Sub- Cycling in Particle Simulation of Plasma	229
DWIN S. CAMPBELL AND MIHALY MEZEI. Torque Algorithms: The Permanent Multipole and Induced Dipole Vector Contributions in a Set of Charge Distributions	245
W. CRYER, P. M. FLANDERS, D. J. HUNT, S. F. REDDAWAY, AND J. STANSBURY. The Solution of Linear Complementarity Problems on an Array Processor	258
HOMAS E. BOOTH. Regional Monte Carlo Solution of Elliptic Partial Differential Equations	281

OTES

FRANZ J. VESELY. Angular Monte Carlo Integration Using Quaternion Parameters: A Spherical Reference Potential for CCl_4	291
---	-----

A. NISHIGUCHI AND T. YABE. Finite-Sized Fluid Particle in a Nonuniform Moving Grid	29
JOHN C. STRIKWERDA. Upwind Differencing, False Scaling, and Nonphysical Solutions to the Driven Cavity Problem	30
HARRY KRUTTER. Numerical Integration of the Thomas-Fermi Equation from Zero to Infinity	30
K. W. KRATKY AND W. SCHREINER. Computational Techniques for Spherical Boundary Conditions	31
R. VAN DOOREN AND J. VLASSENBROECK. Chebyshev Series Solution of the Controlled Duffing Oscillator	32
LIST OF FORTHCOMING ARTICLES	33

NUMBER 3, SEPTEMBER 1982

PETER R. EISEMAN. Coordinate Generation with Precise Controls over Mesh Properties	33
PETER R. EISEMAN. High Level Continuity for Coordinate Generation with Precise Controls	35
HEATHER L. GORDON, STUART M. ROTHSTEIN, AND TIMOTHY R. PROCTOR. Efficient Variance-Reduction Transformations for the Simulation of a Ratio of Two Means: Application to Quantum Monte Carlo Simulations	37
DANIEL R. LYNCH. Unified Approach to Simulation on Deforming Elements with Application to Phase Change Problems	38
M. D. FEIT, J. A. FLECK, JR., AND A. STEIGER. Solution of the Schrödinger Equation by a Spectral Method	41
J.-P. LANQUART. Error Attenuation in Abel Inversion	43
SØREN TOXVAERD. A New Algorithm for Molecular Dynamics Calculations	44
DOUGLAS S. HARNED. Quasineutral Hybrid Simulation of Macroscopic Plasma Phenomena	45
J. B. BELL, G. R. SHUBIN, AND A. B. STEPHENS. A Segmentation Approach to Grid Generation Using Biharmonics	46

NOTES

HENRY E. FETTIS AND ROBERT L. PEXTON. More on the Calculation of Oscillatory Integrals	47
ANDRÉ HAUTOT. Application of Generalized Padé Approximants to the Special Function Evaluation Problem	47
SAMUEL PAOLUCCI AND DONALD R. CHENOWETH. Stability of the Explicit Finite Differenced Transport Equation	48

LIST OF FORTHCOMING ARTICLES

AUTHOR INDEX FOR VOLUME 47

29
30
30
31
32
33
33
35
37
38
41
43
44
45
46
47
47
48
49
49

Journal of Computational Physics

INFORMATION FOR AUTHORS

Articles

The purpose of the *Journal of Computational Physics* is to publish articles concerning techniques developed in the solution of data handling problems and mathematical equations, both arising in the description of physical phenomena.

Manuscripts should be submitted to: *Journal of Computational Physics*, Lawrence Livermore National Laboratory, University of California, P. O. Box 5509, L-561, Livermore, California, 94550.

Original papers only will be considered. Manuscripts are accepted for review with the understanding that the same work has not been and will not be published nor is presently submitted elsewhere, and that all persons listed as authors have given their approval for the submission of the paper; further, that any person cited as a source of personal communications has approved such citation. Written authorization may be required at the Editor's discretion. Articles and any other material published in the *Journal of Computational Physics* represent the opinions of the author(s) and should not be construed to reflect the opinions of the Editor(s) and the Publisher.

Authors submitting a manuscript do so on the understanding that if it is accepted for publication, copyright in the article, including the right to reproduce the article in all forms and media, shall be assigned exclusively to the Publisher. The Publisher will not refuse any reasonable request by the author for permission to reproduce any of his or her contributions to the journal.

Form of Manuscript. Manuscripts should be typewritten with wide margins on high quality 5 × 11 bond paper, using double spacing throughout. The original and two copies should be submitted; however, in order to expedite handling of manuscripts, the original and four copies would be desirable. Copies should include figures and tables.

Each page of the manuscript should be numbered. The first should contain the article title, author and coauthor names and complete affiliation(s). At the bottom of this page, the number of manuscript pages, figures, and tables should be noted. The second page should contain a proposed running head of less than thirty-five characters. It should also contain the name and complete mailing address of the person to whom proofs are to be sent.

With the exceptions noted below, authors should be guided by the Style Manual of the American Institute of Physics.

Subject Classification. As of January 1981 authors are required to classify their own manuscripts using the 1980 *Mathematics Subject Classification*, reprinted from the 1978 *Mathematical Reviews Index*, pp. S27-S34, with the additional classifications listed in the January 1, 1981 issue. Authors are requested to choose at least two categories, one in numerical analysis category, 65, and the other, generally a physical classification, from the categories beyond 65. Page one should contain at least two such classification index numbers.

Abstract. Page 3 should contain a short abstract.

List of Symbols. It is of vital importance that the author submit a complete list of symbols. The symbols used should be identified for the typesetter phonetically. This list will not appear in print, but is essential to avoid costly corrections in proof.

Tables. Number tables consecutively with Roman numerals. Extensive tables will be reproduced as photoengravings, and should be typed carefully in the exact format desired. Authors will be charged for any new engravings necessitated by changes in proof. Use superscript lower-case italic letters (*a*, *b*, *c*) for table footnotes, which should be typed immediately below the table. Type tables at least double-spaced, including titles and footnotes. Do not underline table titles; reserve underlining for text that is to be *italicized*.

Equations. Equations should be typewritten whenever possible, and the number placed in parentheses at the right margin. Reference to equations should use the form "Eq. (3)" or simply "(3)". Superscripts and subscripts should be typed or handwritten clearly above and below the line, respectively. Use the exponent $1/2$ whenever possible.

References. References should be cited in the text by a number in square brackets. Literature cited should appear on a separate page at the end of the article, and should be styled and punctuated according to the following examples:

1. J. G. DEE, *Ann. Phys.* **61** (1969), 880.
[Underline only names of journals.]
2. R. P. SHUTT, "Bubble and Spark Chambers," Vol. 2, p. 50, Academic Press, New York/London, 1967.
3. W. B. THOMPSON, Kinetic Theory of Plasma, in "Advanced Plasma Theory" (M. N. Rosenbluth, ed.), Chap. 1, Academic Press, New York, 1964.

For unpublished lectures or symposia, include title of the paper, name of the sponsoring society full, and date. For journal names, follow the style of Chemical Abstracts' *Service Source Index*. Abbreviation of AEC Laboratory Report names should follow the style of *Nuclear Science Abstracts*.

Footnotes. Footnotes in the text should be avoided if at all possible. If they must be used identify by superscript numbers and type together on a separate page, double spaced.

Figures. All illustrations are to be considered as figures. Number each graph or drawing in sequence with Arabic numerals. Supply a descriptive legend for each figure. Type legends double spaced consecutively on a separate page. The original figures are required. Copies are unacceptable.

Plan figures to fit the proportion of the printed page. Use a professional lettering set on the original so that the letters and numbers are large enough and "open" enough to take a reduction of 50 to 60 % without filling in with ink. Do not include background grids; however, on paper with blue lines the grid can be eliminated in the process of photoreproduction. Identify each figure in a margin with the name of the journal, author's name, and figure numbers; avoid marking the back of figures.

Proofs. Galley proofs will be sent to the author with a reprint order form. Authors will be charged for alterations in excess of 10 % of the cost of composition.

Reprints. Fifty reprints without covers will be provided free of charge. Additional reprints may be purchased.

Notes

Short notes regarding the availability of interesting and useful new programs or tabular material will be considered for publication. Letters to the Editor commenting on articles already published in this Journal will also be considered. Neither notes nor letters should have an abstract.

Probability and Mathematical Statistics: A Series of Monographs and Textbooks

Spectral Analysis and Time Series

Volume 1: Univariate Series

Volume 2: Multivariate Series

edited by M.B. Priestley

Volume 1: May 1981, xx + 702pp., £49.60 (UK only) / \$119.50, 0.12.564901.0

Volume 2: May 1981, xx + 274pp., £20.60 (UK only) / \$49.50, 0.12.564902.9

The book places a special emphasis on the role of spectral analysis, which is closely intertwined with the "time domain" approach. The inclusion of material on "Kalman filtering", "state-space filtering" and "non-linear models" — published here in book form for the first time — and the unusually full treatment of "continuous time" models completes an impressive list of features that will give these two volumes a prominent position among the related literature.

Computational Mathematics and Applications

Analysis of Global Expansion Methods

Weakly Asymptotically Diagonal Systems

edited by L.M. Delves and T.L. Freeman

July/August 1981, x + 276pp., £20.40 (UK only) / \$49.00, 0.12.208880.8

The concept and study of *Weakly Asymptotically Diagonal* (W.A.D.) matrices grew out of an attempt to provide a framework within which realistic *a priori* and *a posteriori* error estimates could be provided for global expansion methods, via a study of the structure of the defining equations for such methods. This study, however, has also led to improved algorithms for handling such equations, and hence has led to considerable advances in methods of implementing global expansion methods. This book brings together, in a coherent form, the results of these studies.

Academic
Press

APL 1193



A Subsidiary of Harcourt Brace Jovanovich, Publishers
London New York Toronto Sydney San Francisco
24-28 Oval Road, London NW1 7DX, England
111 Fifth Avenue, New York, NY 10003, USA

Books to enrich the classroom from Academic Press...

Quantum Mechanics in Hilbert Space

Second Edition

EDUARD PRUGOVEČKI

*A volume in the PURE AND APPLIED
MATHEMATICS series*

This volume provides a rigorous mathematical treatment of the basic aspects of nonrelativistic quantum mechanics. With the exception of group theory, this book treats all the topics covered in standard textbooks on quantum mechanics as well as all the mathematical topics essential to a rigorous approach: basic Hilbert space theory; measure theory and wave mechanics; operator theory; general quantum theory; and quantum scattering theory. This self-contained work presupposes only a general knowledge of calculus and linear algebra. It can serve as an excellent mathematical supplement to intermediate- and advanced-level textbooks on general quantum theory. It can also be used as a textbook for graduate courses on functional analytic methods in quantum mechanics. The key references in the bibliography introduce students to contemporary research problems in various areas of mathematical physics, including quantum scattering theory.

1981, 688 pp., \$39.50 ISBN: 0-12-566060-X

Functional Integration and Quantum Physics

BARRY SIMON

*A volume in the PURE AND APPLIED
MATHEMATICS series*

"Barry Simon has done more than his share producing books that are timely and provide entry to avenues of current research. This book is no exception."

—PHYSICS TODAY

"The author has an extraordinarily secure command of a vast and complex literature, and writes with exceptional clarity and informal charm. The bibliography is . . . quite detailed, and the production is first class. An invaluable addition to the literature of mathematical physics."—SCI TECH BOOK NEWS

This book describes the applications of Brownian motion to proving results in nonrelativistic quantum mechanics. It includes an introduction to the theory of Brownian motion and to a variety of its applications for detailed estimates in quantum theory.

1979, 320 pp., \$37.50 ISBN: 0-12-644250-9 213208

Quantum Mechanics for Applied Physics and Engineering

ALBERT THOMAS FROMHOLD, JR.

An elementary self-contained treatment of the fundamentals of quantum mechanics for undergraduate students in physics and engineering and first year graduate students in engineering and material science. The book presents those aspects necessary for understanding solid state theory, such as quantum statistics and scattering theory.

1981, 448 pp., \$34.00 ISBN: 0-12-269150-4

Qualitative Analysis of Physical Problems

M. GITTERMAN and V. HALPERN

This informative work presents five general principles used in the analysis of physical problems, including the construction of models, dimension analysis, symmetry, analytical properties, and the small parameter method. It features numerous examples that demonstrate the use of these methods in such fields as statistical physics, classical and quantum mechanics, solid state physics, and electrodynamics.

1981, 288 pp., \$24.50 ISBN: 0-12-285150-1

Methods of Modern Mathematical Physics

Volume 1: FUNCTIONAL ANALYSIS

Revised and Enlarged Edition

MICHAEL REED and BARRY SIMON

FROM THE PREFACE TO THE REVISED AND ENLARGED EDITION: "This book is the first of a multivolume series devoted to an exposition of functional analysis methods in modern mathematical physics. It describes the fundamental principles of functional analysis and is essentially self-contained, although there are occasional references to later volumes . . .

This . . . edition differs from the first in two major ways. First, many colleagues have suggested to us that it would be nice to include some material on the Fourier transform in Volume 1 so that this important topic can be conveniently included in a standard functional analysis course using this book . . . Secondly, we have included a variety of supplementary material at the end of the book. Some of these supplementary sections provide proofs of theorems in Chapters II–IV which were omitted in the first edition. . . . Other supplementary sections provide expository material to aid the instructor and the student (for example, "Applications of Compact Operators"). Still other sections introduce and develop new material (for example, "Minimization Functionals").

1980, 416 pp., \$26.00 ISBN: 0-12-585050-6

Send payment with order and save postage and handling. Prices are in U.S. dollars and are subject to change without notice.

ACADEMIC PRESS, INC.

*A Subsidiary of Harcourt Brace Jovanovich, Publishers
New York • London • Toronto • Sydney • San Francisco
111 FIFTH AVENUE, NEW YORK, N.Y. 10003*

Qualitative Analysis of Physical Problems

M. GITTERMAN and V. HALPERN

This informative work presents five general principles used in the analysis of physical problems, including the construction of models, dimensional analysis, symmetry, analytical properties, and the small parameter method. It features numerous examples that demonstrate the use of these methods in such fields as statistical physics, classical and quantum mechanics, solid state physics, and electrodynamics. Each of the principles is considered in a separate chapter. The chapters begin with extensive introductions that provide a review of the topics under discussion. The introductions present simple examples that illustrate applications of the principles. In subsequent sections, these principles are examined and developed in more detail, and their applications to more complex problems are described. Sets of problems are presented at the end of each chapter and, for most of the solutions, references are given to scientific journals.

1981, 288 pp., \$24.50 ISBN: 0-12-285150-1

Send payment with order and save postage and handling.

Prices are in U.S. dollars and are subject to change without notice.

ACADEMIC PRESS, INC.

A Subsidiary of Harcourt Brace Jovanovich, Publishers

New York • London • Toronto • Sydney • San Francisco

111 FIFTH AVENUE, NEW YORK, N.Y. 10003



213207

How To Comply With The New Copyright Law

Libraries everywhere have found the easy way to fill photocopy requests legally and instantly, without the need to seek permissions, from this and over 3000 other key publications in business, science, humanities, and social science.

Participation in the Copyright Clearance Center (CCC) assures you of legal photocopying at the moment of need. You can:

Fill requests for multiple copies, interlibrary loan (beyond the CONTU guidelines), and reserve desk without fear of copyright infringement.

Supply copies simply and easily from registered publications. The CCC's flexible reporting system accepts photocopying reports and returns an itemized invoice. You need not keep any records, our computer will do it for you.

The Copyright Clearance Center is your one-stop place for on-the-spot clearance to photocopy for internal use. You will never have to decline a photocopy request or wonder about compliance with the law for any publication registered with the CCC.

For more information, just contact:



Copyright Clearance Center

21 Congress Street
Salem, Massachusetts 01970
(617) 744-3350

a not-for-profit corporation

NAME _____ TITLE _____

ORGANIZATION _____

ADDRESS _____

CITY _____ STATE _____ ZIP _____

COUNTRY _____ TELEPHONE _____